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Three-Body Dynamics in Single Ionization of Atomic Hydrogen by 75 keV Proton Impact

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Doubly differential cross sections for single ionization of atomic hydrogen by 75 keV proton impact have been measured and calculated as a function of the projectile scattering angle and energy loss. This pure three-body collision system represents a fundamental test case for the study of the reaction dynamics in few-body systems. A comparison between theory and experiment reveals that three-body dynamics is important at all scattering angles and that an accurate description of the role of the projectile–target-nucleus interaction remains a major challenge to theory.

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Studies of atomic fragmentation processes, such as ionization of atoms by charged particle impact, are of fundamental importance since they directly address the yet unsolved few-body problem [1,2]. Because the Schrödinger equation is not analytically solvable for more than two mutually interacting particles, theory has to resort to heavy numerical modeling efforts. Calculations of reaction cross sections are thus very challenging even for the simplest collision systems involving only three particles.

In the case of electron-impact ionization, major progress in describing the reaction dynamics has been achieved in the past decade. Sophisticated nonperturbative models were developed which treat the entire collision system, including the projectile, quantum-mechanically (e.g., [2–4]). However, for ion impact, treating the projectile accurately is much more challenging because a large number of angular momentum states contribute to the scattered wave as a result of the large projectile mass. Recently, nonperturbative methods were reported for ion impact as well; however, they do not account for the interaction between the projectile and the target nucleus (*NN* interaction) [5,6]. Only perturbative approaches accounting for the *NN* interaction in an approximate manner are available for ion-impact ionization (e.g., [7–9]). Nevertheless, these models were believed to provide an adequate description of the collision dynamics at least for collision systems with not too large perturbation parameters η (projectile charge to velocity ratio). However, the surprising observation of qualitative discrepancies between experiment and theory for η as small as 0.1 [1] showed that for ion impact, theory is still facing significant problems.

Because of these difficulties, accurate and detailed experimental benchmark data are essential for theoretical modeling efforts. Ionization of atomic hydrogen by electron or bare ion impact, i.e., a pure three-body system, constitutes a particularly important test case. As this represents the simplest collision system pertaining to the few-body problem, it is the most suitable test of the fundamental components of theoretical models. For heavier target atoms, the presence of passive electrons, i.e., those not undergoing a transition, means that in the calculation a significantly more complex target wave function has to be used, for both the initial and the final state. Although to find a sufficiently accurate wave function is usually not too problematic, using it within a complex scattering amplitude can make the calculation of cross sections numerically much more complicated. As a result, measurements for heavier target atoms may provide a test on the numerical accuracy of the electronic wave function, but they are not ideally suited to test the basic description of the reaction dynamics.

Experiments using an atomic hydrogen target are much more challenging than, e.g., a noble gas or molecular gas target because of the need to efficiently dissociate molecular hydrogen. Although an extensive literature exists on total cross section measurements for capture from (e.g., [10–12]), excitation of (e.g., [13,14]), and ionization of atomic hydrogen (e.g., [15–17]), differential measurements are much rarer (e.g., [18–22]). Ion-impact measurements differential in projectile parameters are particularly difficult because the scattering angle θ_p and the energy loss ΔE (relative to the total energy) are usually very small. A simultaneous measurement of both quantities with sufficient resolution is very difficult even for a helium target and has been reported by one group only using a unique high-resolution projectile energy-loss spectrometer [23]. For an atomic hydrogen target, one is confronted with the additional problems associated to the need to dissociate molecular hydrogen, such as a much smaller target density compared to helium. Furthermore, because of the imperfect dissociation, the projectiles have to be measured in coincidence with the recoil ions in order to separate H^+ from $H_2{}^+$ and from residual-gas background. Because of these difficulties, only single differential cross sections as a function of θ_p for capture [19] and excitation [20] and as a function of ΔE for ionization [21] have been reported.

Measured data on double differential cross sections (DDCS) as a function of both θ_p and ΔE (or equivalently electron energy) for ionization of atomic hydrogen by ion impact do not exist. Only for electron impact, for which θ_p and ΔE are much easier to measure, are experimental multiple differential cross sections as a function of projectile parameters available (e.g., [24,25]). However, these measurements are restricted to relatively small projectile energies, where significant differences between the ionization cross sections for electron and ion impact are expected [26].

In this Letter, we report the first measurements of DDCS as a function of θ_p and ΔE for ionization of atomic hydrogen by ion impact. These data represent the most sensitive test case of the theoretical description of the collision dynamics in a pure three-body system currently available. The comparison with theory confirms that difficulties of various theoretical models to reproduce earlier experimental data for ionization of helium by ion impact are not just caused by the complexity of the initial target state but are due to an insufficiently accurate description of the few-body dynamics of the active particles.

The experiment was performed at the Missouri University of Science and Technology. A 5 keV proton beam was generated from a hot cathode ion source, accelerated to 75 keV, and collimated by a set of slits 0.1 mm by 0.1 mm in size. A neutral atomic hydrogen beam was generated using a microwave dissociator. After exiting the discharge region, the hydrogen gas was guided through Teflon tubing to a Teflon-coated glass needle. The target beam was then collimated by a skimmer, also made out of Teflon, and was crossed with the proton beam. This collimation cools the target beam in the plane perpendicular to the direction of expansion to a temperature of 1–2 K. Parallel to the expansion, cooling is achieved by adiabatic expansion due to the pressure gradient between the region inside the needle (≈ 0.4 Torr) and the surrounding region, which is kept at about 1×10^{-6} Torr by a turbo pump. In this direction, the temperature is significantly higher (5–10 K). Cooling of the target (which is needed in future experiments) is achieved at the expense of a reduced degree of dissociation (see also [22]). At the intersection with the projectile beam, the target beam was measured to contain approximately 30%–40% atomic and 60%–70% molecular hydrogen.

The recoil ions were extracted by a weak electric field (≈ 5 V/cm) pointing perpendicular to the projectile beam direction and detected by a two-dimensional position-sensitive channel-plate detector. The scattered projectiles were charge-separated by a switching magnet, and the proton component was decelerated to an energy of 5 keV. A parallel plate analyzer [27] was used to measure the energy loss the protons suffered in the collision with the target. The projectile detector was also equipped with a two-dimensional position-sensitive anode so that all θ_p were measured simultaneously in a single data run. However, the entrance and exit slits of our energy analyzer restricted recording of data to only one ΔE at a time. The overall energy-loss resolution (including the energy spread of the projectile beam of less than 1 eV [27]) was 3 eV full width at half maximum (FWHM), and the resolution in θ_p was better than 0.1 mrad FWHM. The recoil-ion and projectile detectors were set in coincidence. In the coincidence time spectrum, different ion species are separated by their charge-to-mass ratio. H_2^+ ions resulting from ionization of the nondissociated target gas component therefore do not contaminate the measurement for atomic hydrogen.

The coincident projectile position spectrum is proportional to the double differential cross section DDCS $= d^2\sigma(\theta_p, \Delta E)/d\Omega_p d(\Delta E)$, where Ω_p is the projectile solid angle. For normalization purposes, single differential cross sections SDCS $= d\sigma/d(\Delta E)$ of Park *et al.* [21] were used. Their total cross section, obtained from the integral of the SDCS, is too large by about a factor of 1.8 compared to recommended data [28]. We therefore normalized our DDCS integrated over Ω_p to the SDCS of Park *et al.* divided by that factor. At ΔE larger than 45 eV, no measured data are available. Up to that energy, the data of Park *et al.* divided by 1.8 are exactly a factor of 2 smaller than the corresponding cross sections for H_2. At larger ΔE, we thus normalized our DDCS to half the SDCS for H_2 [29].

In Fig. 1, the measured DDCS are plotted as a function of θ_p for fixed ΔE of 30, 40, and 50 eV. The horizontal error bars indicate the bin size over which θ_p was averaged; however, the accuracy in θ_p is much better than suggested by these error bars. The dotted curves show our continuum-distorted-wave–eikonal-initial-state (CDW-EIS) calculation, which does not account for the *NN* interaction [9]. The theoretical results were convoluted with the experimental resolution in both ΔE and θ_p using a Monte Carlo simulation [30]. Only for $\theta_p \leq 0.1$ mrad was a small effect due to the resolution found. Somewhat unexpectedly, the CDW-EIS results exhibit a slight maximum at $\theta_p \approx 0.2$ to 0.3 mrad (depending on ΔE). In the first Born approximation [(FBA), dashed-crossed curves] at $\Delta E = 50$ eV this maximum is even more pronounced. It can be explained in terms of binary interactions between the projectile and the electron in which the recoiling target nucleus remains essentially at rest (and we thus label this structure a ''binary peak''). For such two-body kinematics, θ_p is readily determined by ΔE. For p + He collisions at the same projectile energy, in contrast, the DDCS in the FBA just fall off monotonically without any structure [7,23] because the two-body kinematics is ''washed out'' by the much broader initial momentum distribution of an electron bound in helium compared to hydrogen.

The binary peak in the CDW-EIS calculation is not seen in the present data, and its agreement with our experimental data is not very good. Although at intermediate θ_p (approximately 0.2–0.6 mrad) the agreement is not bad, large discrepancies are found at θ_p smaller than 0.2 mrad

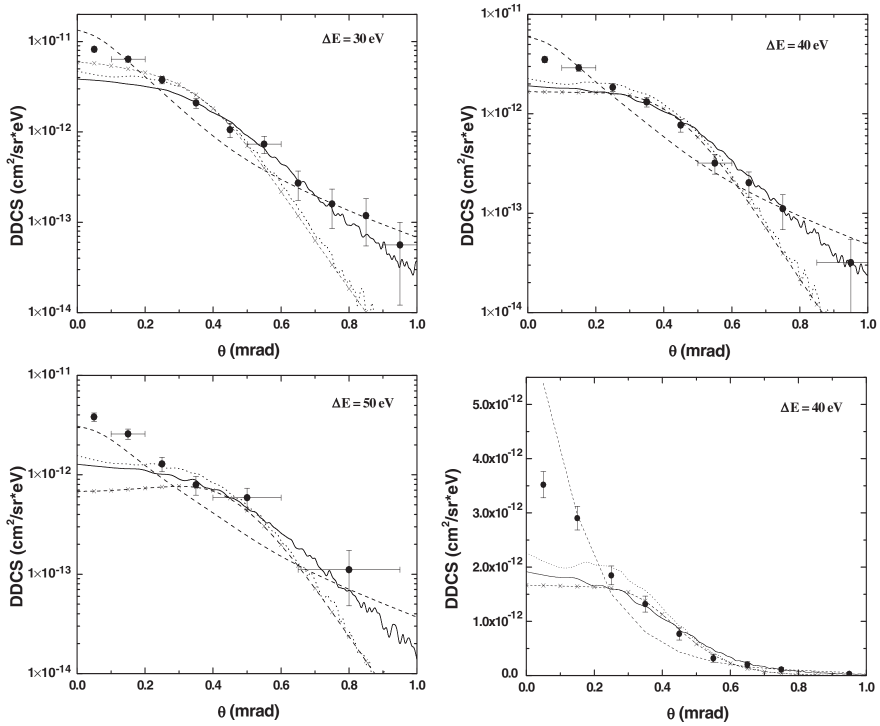

FIG. 1. DDCS plotted as a function of the projectile scattering angle θ_p for fixed energy losses ΔE of 30, 40, and 50 eV, respectively. Dashed-crossed curves, FBA; dotted curves, CDW-EIS; dashed curves, CDW-EIS-NN; solid curves, CDW-EIS convoluted with classical elastic projectile–target-nucleus scattering (see text). The lower right panel shows the DDCS for 40 eV on a linear scale.

and larger than 0.6 mrad. It seems plausible to fault these deviations on the *NN* interaction not accounted for in the CDW-EIS model. The dashed curves in Fig. 1 show a modified CDW-EIS calculation in which the *NN* interaction is accounted for using the eikonal approximation [9], which we label the CDW-EIS-NN model. Disappointingly, this calculation leads to only marginally improved agreement with the data. Although improved agreement is achieved at small and large θ_p, the price to be paid is that considerable discrepancies now occur at the intermediate angles where the CDW-EIS model fared quite well.

The solid curves in Fig. 1 show calculations in which the CDW-EIS cross sections were convoluted with classical elastic scattering between the projectile and the residual target ion. This convolution, which we label CDW-EIS-CLNN, was performed with the same Monte Carlo simulation that was used for the convolution with the experimental resolution (for details, see [30,31]). The CDW-EIS-CLNN calculation is in essentially perfect agreement with the DDCS data for $\theta_p > 0.2$ mrad. Only for very small θ_p does the CDW-EIS-NN model, i.e., the quantum-mechanical treatment of the *NN* interaction, seem to work somewhat better (a more detailed comparison in this region is discussed below).

It is well known that for deflection of a proton from a free electron there is a maximum scattering angle of about 0.55 mrad [32]. Larger scattering angles in ionization of atoms must therefore be either due to the bond of the electron in the initial target ground state or due to additional deflection of the projectile from the target nucleus. Since regardless of scattering angle any electronic transition from the ground state always requires an interaction between the projectile and the electron, ionization is expected to be dominated by three-body dynamics at large θ_p. This is indeed supported by the much better agreement of the present data with the calculations with compared to those without *NN* interaction. At $\theta_p < 0.55$ mrad, on the other hand, ionization due to a binary projectile-electron interaction is kinematically possible. At small scattering angles the role of three-body dynamics is thus not immediately clear. To address this question by comparing experiment to theory, a semilogarithmic presentation of the DDCS, which is necessary to present the θ_p dependence over the entire measured angular range, is not ideally suited. For a more detailed comparison at small θ_p, we therefore present the DDCS for $\Delta E = 40$ eV on a linear scale (for the other energy losses, the comparison between theory and experiment is similar) in the lower right panel in Fig. 1.

The spectrum with the linear scale shows some features more clearly which are not as prominent on the semilogarithmic scale. First, it now becomes more evident that even for $\theta_p < 0.2$ mrad there are considerable discrepancies (around 50%) between the CDW-EIS-NN calculation and the data. These very small scattering angles thus seem to represent the most challenging region for theory to accurately treat the three-body dynamics since none of the calculations is in good agreement with the data. Second, the comparison between the CDW-EIS and CDW-EIS-NN models shows that in the latter the binary peak is "washed out" by elastic projectile–target-nucleus scattering. To a much lesser extent this is also true for the CDW-EIS-CLNN calculation. However, it follows the trend of the CDW-EIS results at intermediate θ_p insofar as a slight "shoulder structure" remains, in accord with the data. Overall, the present results suggest that three-body dynamics plays an important role at all scattering angles.

A similar comparison between experiment and theory was also observed for 100 MeV/amu C^{6+} + He collisions: There, too, the data seemed to favor a classical description of the *NN* interaction over the quantum-mechanical treatment [31]. Indications for theoretical difficulties to accurately account for the *NN* interaction quantum-mechanically were also found in other collision systems (e.g., [33,34]). Obviously, this does not mean that a classical approach is generally more adequate than a quantum-mechanical treatment, but it does mean that the specific methods used so far to incorporate the *NN* interaction in perturbative calculations is not accurate enough. In spite of the partial success of the classical treatment of the *NN* interaction, the three-body dynamics in simple atomic systems can be considered as understood only if satisfactory agreement with experimental data is obtained consistently with a fully quantum-mechanical approach. As mentioned above, nonperturbative methods applied to electron-impact ionization were much more successful, although even there non-negligible discrepancies to measured data for ionization of helium remain [35]. Nevertheless, for ion impact, too, it seems necessary to develop nonperturbative methods accounting for the *NN* interaction quantum-mechanically. Such efforts are currently underway.

In summary, we have for the first time measured DDCS as a function of the projectile scattering angle and energy loss for ionization of atomic hydrogen by ion impact. Such pure three-body collision systems offer a much more sensitive test of the theoretical description of the few-body dynamics because uncertainties introduced by more complex initial-state wave functions of many-electron targets are removed. The comparison between theory and experiment reinforces that our understanding of even three-body dynamics is still incomplete. In particular, an accurate treatment of the *NN* interaction remains a major challenge to theory.

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